

Diethyl ether

60-29-7 | DTXSID3021720

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $9.74 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $7.68 \times 10^{-1}$

**Confidence level:**  $6.64 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Diethyl ether

**Measured:**  $1.31 \times 10^{-11}$

**Predicted:**  $9.74 \times 10^{-12}$

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Tetrahydrofuran

**Measured:**  $1.61 \times 10^{-11}$

**Predicted:**  $7.41 \times 10^{-12}$

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Tetrahydropyran

**Measured:**  $1.38 \times 10^{-11}$

**Predicted:**  $9.55 \times 10^{-12}$

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1,2-Epoxybutane

**Measured:**  $1.91 \times 10^{-12}$

**Predicted:**  $5.74 \times 10^{-12}$

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Isopropanol

**Measured:**  $5.07 \times 10^{-12}$

**Predicted:**  $5.72 \times 10^{-12}$